Chemistry and Organics Working Groups

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Working Group Meetings:
Emissions and Deposition: Wednesday 3:00 – 4:15, Room MD119
Chemistry: Thursday 9:00 – 10:15, Room G115
GEOS-Chem may be a bit light on gas phase tracers, but we can’t add them all. What/where are the priorities?

Theoretically, the problem could be much worse. To fully describe oxidation: $10^4 - 10^{10}$
One common research theme across these WGs is constraining emissions.

Over North America...

And India...

See Poster A.6  (Sreelekha Chaliyakunnel, U. Minnesota)

See Poster A.8  (Xin Chen, U. Minnesota)

See Poster B.23  (Zitely Tzompa, CSU)

New NEI implementation
There is a dicarbonyl simulation and adjoint, and its been used in a full adjoint inversion for Chinese and global VOC emissions.

See Poster A.7

Hansen Cao and Tzung-May Fu, Peking Univ.
The model has also been used to derive surface HCHO mixing ratios, and quantify implications for health.

![OMI-derived mean HCHO in surface air and cancer risk](image)

6600–13200 people in the US will develop cancer over their lifetimes by exposure to outdoor HCHO.

*Lei Zhu, Harvard.*
We have new strategies for setting research priorities, e.g. Morris Method. What uncertainties matter for which questions?

Talk at 4:30 today

Jared Brewer, CSU.
Updates have led to more active tropospheric ozone chemistry, and the best simulations yet.

A. Update anthropogenic emissions
B. Better constrained lightning NO\textsubscript{x} location
C. Add Br chemistry
D. Decreased NO\textsubscript{x} sink from isoprene nitrates
E. Change in GEOS meteorological field
F. I,Br, Cl chemistry V11.2

Talk at 3:00 today
Hu et al. Atmos. Environ. In review
But, a Monte Carlo ensemble on inorganic rate constants shows that chemical uncertainties on what we know best are still large.

Figure 4. Spatial distribution of uncertainties.

Fractional uncertainties calculated for $\text{O}_3$, OH and CO concentrations for the tropospheric column (left), the zonal mean (centre) and the surface (right) from adding together the individual reaction uncertainties from the 60 reactions studied in quadrature.

Ben Newsome, ACPD, University of York
Halogenso have a big impact on troposphere.

Br: Parrella et al., 2012 V9
Br+Cl: Schmidt et al., 2016
I: Sherwen et al., 2016a
I+Br+Cl: Sherwen et al., 2016b

Trying to include I+Br+Cl in V11.2

Talk from Mat Evans 2:30.
Sherwen et al., ACP, 2016
FLEXChem arrived in V11. This is a BIG change to the representation of the chemistry.

• From GEOS-Chem V1 we used globchem.dat and SMVGear to describe the chemistry.

• From V8 we had KPP and SMVGear running simultaneously. This was rather inelegant.

• For V11 we have a clean implementation of KPP within the model thanks to Mike Long and the support team.

• Need to have all diagnostics – concentrations, fluxes, rate constants working and efficient.
There are many recent updates that overlap the Chemistry and Organics working groups.

**v11.1 Error Corrections / Updates**
- PMN + O₃ → Update products       Dylan Millet
- MOBA + OH → MOBAOO              Will Porter
- ISNOAA + NO₂ → PMN              Mike Long
- Fix molecular weight of N₂O₅    Chi Li

**v11.1 New Science**
- Criegee intermediates           Dylan Millet

**v11.1 New Engineering**
- FlexChem                        Mike Long

**v11.2 Error Corrections / Updates**
- JPL 15 Barron Henderson / Thomas Sherwen
- ALK4 lumping                    Barron Henderson
- Monthly mean NEI2011            GCST / Katie Travis

**v11.2 New Science**
- PAN Updates                     Emily Fischer
- Isoprene nitrates updates       Jenny Fisher / Eloise Marais / Kelvin Bates / Katie Travis
- I, Br, Cl Trop Chemistry        Tomas Sherwen
These are the updates relevant to Emissions & Deposition that are also slated for v11.2.

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<th>v11.2 Error Corrections / Updates</th>
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<td>EDGAR v4.3 emissions</td>
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<td>Arctic seabird NH₃ emissions</td>
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<td>NOₓ from snowpack</td>
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<td>Non-agricultural NH₃</td>
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This is the new working group structure, and your chairs.

Emissions & Deposition Working Group

- Jintai Lin
- Eloise Marais
- Dylan Millet
- Emily Fischer

Chemistry Working Group

- Mat Evans
- Barron Henderson
- Lu Hu
- Jingqiu Mao
We have much to discuss during the breakout sessions. Emissions and Deposition Topics:

• Should bi-directional fluxes be prioritized?

• Are parameterizations of fire plume injection heights ready for global application?

• What are emerging issues for prioritization? Which emerging issues are your highest priorities? Which will provide the most benefit to the broader community?

• Other questions/challenges?
Among others, the Chemistry WG is planning on discussing these questions?

• As we extend the hydrocarbons (i.e. terpenes, aromatics, larger VOCs), how should we handle speciation?

• Should we be moving all chemistry to KPP (e.g., lumped monoterpenes)?

• What are emerging issues for prioritization? Which emerging issues are your highest priorities? Which will provide the most benefit to the broader community?

• Other questions/challenges?

Chemistry:
Thursday 9:00 – 10:15, Room G115